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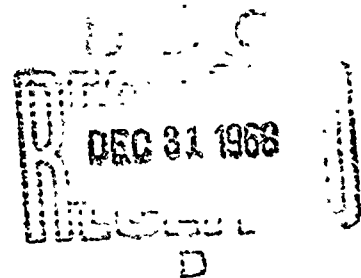
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SOME STRONG WAVE PROBLEMS IN AN ELASTIC MATERIAL WITH MICROSTRUCTURE

by

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ABSTRACT

The historical development of the foundations of thermomechanics is reviewed, with emphasis placed upon the critical contribution of each investigator. The theories are discussed in terms of their relevance to real materials in the important high-velocity regime which lies between the low and intermediate velocity regime (which involves essentially isothermal elastic and plastic wave propagation) on one hand and the ultrahigh-velocity regime (in which a hydrodynamic description of the material behavior is adequate) on the other. Various facets of high-velocity wave propagation in various materials involve elastic, plastic, viscous, and thermal effects on a macroscopic scale and perhaps on a microscopic scale. Evaluations are made from the standpoint of thermodynamics as well as classical mechanics.

Using fundamental principles of thermodynamics and mechanics, thermomechanically coupled linear energy and constitutive equations are derived for the elastic solid with microunit cells discussed by Mindlin.

Equations of motion for the microstructure are found for the large amplitude case where Eulerian and Lagrangian formulations are not identical.

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I. REVIEW OF PREVIOUS WORK

A. INTRODUCTION

In the past decade, a very large body of experimental data on the behavior of various solids under strong shock loading has been obtained by means of a variety of high-pressure dynamic loading techniques.^{1,2,3} Since most of the original experimental work was conducted at very high pressures (say, three or more orders of magnitude above the ultimate strength) at which it has been recognized that strength effects are not important, the analyses developed to describe this work mathematically were based on hydrodynamics of dense, inviscid fluids. More recent effort has been devoted to hypervelocity impact (HVI), i.e., the impact of a small body with a massive body at relative velocities exceeding the acoustic velocities of both. Since HVI involves creation of craters of finite size, it must depend upon the strength properties of the materials involved. Most of the attempts to analyze HVI have involved either minor modification of hydrodynamic theory or correlation of highly simplified phenomenological models with experimental results.

An example of the inadequacy of the hydrodynamic approach for the high-velocity regime has been reported by Curran.⁴ The results of his plate-slap experiments on 2024 aluminum-alloy plates at an impact velocity of 1.9 mm/ μ s indicated that attenuation begins approximately 80-percent sooner and is approximately twice as severe as predicted by hydrodynamic theory. An analysis able to predict this greater attenuation accurately is highly desired.

Until very recently, thermodynamic aspects of high-velocity wave propagation have been highly neglected. Although the theory of linear elastic materials with thermomechanical coupling (through the energy equation) dates back to 1837 with Duhammel's work,⁵ there have been few new major accomplishments in thermomechanics until about ten years ago. Since the topic of linear thermoelasticity without thermomechanical coupling has been treated extensively in Boley and Weiner's textbook,⁶ it is omitted here.

B. THERMOELASTICITY

Although the energy equation and constitutive equations for a classical linear elastic solid with thermomechanical coupling were originated by Duhamel in 1837, surprisingly little work has been done in this area. Here the term "classical" means one without microstructural effects and with elastic properties independent of temperature. Most of the analyses reported in the literature are concerned with the response (thermal and mechanical) due to sudden or cyclic heating but no mechanical loading. It appears that more analysis should be devoted to problems involving purely mechanical loading, with particular emphasis on determining the loading rate at which the thermomechanical coupling effects become important. On a strictly intuitive basis, it is believed that in the regime in which thermomechanical coupling effects become important, the use of a finite description of strain, rather than the linear infinitesimal one, is necessary.

One of the most interesting anomalies in the behavior of a classical, linear elastic solid with thermomechanical coupling has been discussed by Deresiewicz:⁷ His analysis predicted that the phase velocity of plane elastic waves approach the adiabatic value at low frequencies and the isothermal value at high frequencies. Deresiewicz pointed out that this is in disagreement with the Laplace-Rayleigh thermomechanical theory of gases, which Deresiewicz claimed is erroneous.

Although various theories of elasticity,⁸⁻¹⁰ taking into consideration doublet stresses (doublet forces/area) in addition to classical stresses (forces/area), have been proposed to explain such phenomena as size effects in materials and crystal-lattice-type wave dispersion; only recently has attention been given to the thermodynamic aspects of such solids.¹¹⁻¹⁵

In all of the theories of thermoelasticity known to the authors, the temperature dependence of the elastic constants is neglected, even though a recent thermomechanical theory of elastoplastic waves in solids

considers an effect of the same order of magnitude: the effect of temperature on the yield strength.¹⁵ Rosenfield and Averbach,¹⁶ in an analysis which is on a rather weak mathematical and thermodynamic basis, indicated that the temperature dependence of the elastic coefficients is related to the stress dependence of the thermal-expansion coefficient α as follows:

$$\alpha = \alpha_0 + \alpha_1 \sigma \quad (1)$$

where

$$\alpha_1 = -E^{-2} dE/dT \quad (2)$$

where α_0 is the coefficient of thermal (linear) expansion at zero stress, α_1 is the change in this coefficient per unit of normal stress, σ is the normal stress applied in the direction in which α is measured, E is Young's modulus, and T is temperature. Rosenfield and Averbach conducted experiments which confirmed the linear dependence of α with stress, as predicted by Eq. 1. However, the discrepancy between the value of the proportionality constant α_1 predicted by their theory, Eq. 2, and that measured varied from 6 to 100 percent. An analysis which is on a more sound thermodynamic and mathematical basis than that of Ref. 16 is given in the appendix. Unfortunately the new theory requires additional experimental data which are not normally available, namely the variation of α_1 with temperature.

Following a procedure suggested in Boley and Weiner's,⁶ Pilon¹⁷ formulated a theory of thermoelasticity for physically nonlinear elastic solids. He considered the strains as independent thermodynamic variables ("fluxes") and the stresses as dependent thermodynamic variables ("forces"); thus, he utilized the Helmholtz free energy function (also called the Gibbs work function). It appears that he might just as well have considered the stresses as independent variables and the strains as dependent variables, and then utilized the Gibbs thermodynamic potential.¹⁸

Vakulenko¹⁹ has considered stress as the independent thermodynamic variable in his work in thermoplasticity, and Burridge and Knopoff²⁰ have introduced a formulation of mechanical energy, using stress as the independent variable, which is valid for prestressed and inelastic media as well as nonprestressed elastic media. This approach is used in the appendix to considerably simplify the derivation of the stress dependency of the thermal-expansion coefficient.

Another type of nonlinearity, namely geometric nonlinearity (i.e., finite deformations), has been discussed very ably by Lee and Liu,²¹ and some of the underlying thermodynamics aspects have been put on a sound mathematical basis by Coleman and Noll²² and Wang and Bowen.²³

C. THERMOPLASTICITY

The quantitative experiments of Farren and Taylor²⁴ in 1925 form the basis for thermoplasticity. They found that approximately 90 percent of the work done in plastic deformation is dissipated in the form of heat and the remaining 10 percent is irreversibly stored due to permanent distortion of the crystal lattice.

Some of the work in thermoplasticity has been largely of a philosophical nature.²⁵⁻²⁷ The first attempts to put the subject on a quantitative basis were made independently by Freudenthal,²⁸ Prager,²⁹ Ziegler,³⁰ and Vakulenko.^{31,19} Their work has been discussed critically by Naghdi,³² who considered their work strictly exploratory in nature. His primary objection was that their theories are uncoupled, i.e., they do not contain a heat conduction term. He also questioned their choice of state variables and generalization of Onsager's principle to nonlinear phenomena.

Grigorian³³ took the viewpoint that, although thermodynamic concepts are of limited usefulness in constructing the mechanical parts of constitutive equations, one should check the thermodynamic consequences of a tentative constitutive relation in order to make the mathematical model

thermodynamically complete. (This point is illustrated in the consideration in the appendix.) It is interesting to note that Grigorian recognized that some of the plastic work goes into increasing the internal energy due to changes in structure of the material.

Foster³⁴ devoted attention to relaxation-spectrum effects. In particular, he noted that there are different relaxation spectra for loading (increasing load) and unloading (decreasing load).

Assuming that all of the plastic work is dissipated in the form of heat, Dillon³⁵ formulated a theory of thermoplasticity with thermomechanical coupling for small strains and Backman³⁶ formulated an analogous theory for finite strains. However, the latter work has been criticized and improved upon by Lee and Liu.²¹

To date the most complete mathematical models for dynamic thermoplasticity analyses are those of Grigorian³⁷ (with emphasis on soils) and Lee and Wierzbicki¹⁵ (with particular reference to metals).

As mentioned previously, Lee and Wierzbicki¹⁵ included the effect of temperature on the yield strength, but neglected the thermodynamically related effect of stress on the thermal-expansion coefficient, α . In their experiments, Rosenfield and Averbach¹⁶ measured this effect for stresses well into the plastic range. They found that as soon as the elastic limit is exceeded, α increases with stress at a greater slope than in the elastic range. However, the slope decreases with increasing stress, eventually becoming zero, and finally negative. When they removed the stress after each successive loading, they found that the permanent changes in α also increased, then leveled off, and finally decreased at higher applied-stress levels. This appears to be closely related to the observations of Farren and Taylor²⁴ that the percentages of the total plastic work which goes into permanent distortion of the lattice varies with applied strain. In view of these considerations, it

is conjectured that the effect of the stress dependency of the thermal-expansion coefficient would be greatest for short-duration pulses in which the loading is removed before there is sufficient time for very large plastic strains to be reached. However, as in the case of the same effect in the elastic range, quantitative inclusion of this effect in a theory must await experimental measurements of it over a range of temperatures ranging upward from room temperature.

D. THERMOVISCOELASTICITY

The theory of thermoviscoelasticity has strong thermodynamic bases, thanks to extensive research by Biot,³⁸⁻⁴⁰ Chu,⁴¹⁻⁴² Schapery,⁴³⁻⁴⁵ and Coleman.⁴⁶⁻⁴⁸ Other research on the formulation of constitutive equations for thermoviscoelasticity has been carried out by Eringen,⁴⁹ Cowin,⁵⁰ Chudnovskii,⁵¹ and Leigh.⁵²

Various aspects of the nonlinear theory of viscoelasticity have been treated in recent work by Koh and Eringen,⁵³ Kline,⁵⁴ and Valanis.⁵⁵ Recently Eringen⁵⁶ has formulated a theory of microstructural viscoelasticity including thermodynamic considerations.

The literature which has appeared in the past decade on dynamic thermoviscoelastic (DTVE) problems is too voluminous to mention in detail here. For a basic treatment of the subject, reference is made to Boley and Weiner's book.⁶ Most of the DTVE analyses found in the literature neglect thermomechanical coupling. An example of one of the few DTVE analyses in which this coupling is considered is found in Ref. 57.

It appears that the possibility of the type of thermomechanical instability discussed by Berg⁵⁸ should be investigated further, especially for high-intensity waves. He pointed out that the softening of a body due to heating allows external loads to deliver more power to the body at an increasing rate.

E. WAVE PROPAGATION

There are two fundamentally different types of waves:

1. Simple, continuous waves, which can be mathematically described by a Fourier series of harmonic waves. These waves are of small amplitude and are often called acoustic waves.
2. Discontinuous waves which involve a discontinuous jump in some physical quantity. The order, n , of a discontinuous wave is the order of the time derivative of the displacement which is discontinuous. Thus, a shock wave, which involves a jump in velocity, is a first-order wave and is usually the most severe.* Higher order waves involve jumps in acceleration (acceleration waves) and in higher time derivatives.

The classical treatment, as used by Rayleigh,⁵⁹ is adequate for handling acoustic waves. The literature on the propagation of such waves in elastic and viscoelastic solids is too voluminous to mention here except to refer to two texts^{60,61} and three review papers devoted to this topic.⁶²⁻⁶⁴

The common metallic alloys used in load-carrying applications, namely steel, aluminum and most titanium alloys, behave macroscopically as isotropic materials at least in the elastic range. However, since they are really aggregates of many highly anisotropic crystals, they behave anisotropically on a microscale. This has been the motivation for various theoretical⁶⁵⁻⁶⁸ and experimental studies⁶⁹ of acoustic-wave propagation in single crystals. A few metals and alloys of increasing engineering importance, namely beryllium, certain titanium alloys, zirconium, and uranium, are anisotropic even on a macroscale. Furthermore, filamentary composites behave anisotropically on a macroscale.

* An alternative, but equivalent, definition of the order n of a discontinuity is one plus the order of the space derivative of the strain which is discontinuous. Thus, a shock wave, which involves a jump in strain, is a first-order wave.

The development of theories of solids with microstructure^{10,13,14} now permits a mathematical treatment of solids which are isotropic on a macroscale and yet anisotropic on a microscale. This opens a new avenue of improved correlation between theory and experimental studies of acoustic wave propagation. However, to date, studies along this line have been limited to theoretical studies of relatively simple systems.^{10,70-72}

The method of characteristics, which is based on the concept of a characteristic surface or discontinuity surface appears to have been developed at the turn of the century by Hadamard⁷³ for the study of the propagation of discontinuities in hydrodynamics. The method has found wide use in fluid mechanics, including gas dynamics and magnetofluidmechanics as well as hydrodynamics.

Apparently the first application of the method of characteristics to solids behaving nonhydrodynamically is due to Thomas. He was originally concerned with plastic solids⁷⁴ but later generalized his compatibility conditions.⁷⁵⁻⁷⁶ Hill⁷⁷ discussed stability and uniqueness of acceleration waves in general media with emphasis on incompressible and elastoplastic media. Acceleration waves in anisotropic elastic solids were analyzed by Howard,⁷⁸ who was concerned with transversely isotropic media and Nariboli⁷⁹ who treated general anisotropic elastic media. Nariboli's approach is interesting in that he combined the singular surface concept of Thomas with the ray theory of Courant and Hilbert to obtain an equation which upon integration predicts the growth or decay of the discontinuities. Very recently Lur'e⁸⁰ has analyzed the propagation of discontinuities in continuation with microstructure.

Recently a number of investigators⁸¹⁻⁸⁵ have investigated nonlinear aspects of acceleration waves and higher-order waves in nonlinear elastic materials. Some of the general results of these studies are:

1. When the strain has a discontinuity, the derivative of the strain also must have a discontinuity.⁸² Thus, shock waves

(to be discussed later) are accompanied by acceleration waves although the converse situation does not necessarily hold.

2. Varley and Dunwoody⁸³ found that the linear theory of irrational waves has an error which increases with time. Their nonlinear theory predicts that either a shock forms or the material "forgets" the details of the disturbance in a finite time. Green's theory⁸⁴ predicts that acceleration waves either become infinite in finite time (i.e., a shock forms) or decay to zero in infinite time, with the exception of transverse waves normal to a shock.
3. Discontinuities of higher order than the second propagate with constant strength⁸⁴ and at the same velocity as the acceleration wave.⁸⁵

In their book,⁸⁶ Truesdell and Noll presented a review of acceleration waves in generalized elastic media. Recently considerable attention has been devoted to acceleration waves in viscoelastic media.⁸⁷⁻⁹³ Of these, the work of Varley is especially important because the material may be generally anisotropic and nonhomogeneous.

The problem of the propagation of discontinuities into a prestressed medium is important in connection with propagation of unloading waves (if the duration of loading is sufficiently long compared to the transit time of the reflected wave), since then the medium is essentially prestressed by the loading wave. For small deformations (i.e., acoustic waves), this problem was treated by Biot.⁹⁴ The case of acoustic waves but large deformation due to the prestress have been considered in Ref. 95-97. Finally, the propagation of finite discontinuities in prestressed media has been treated by Green.⁹⁸

Although the foregoing analyses employ thermodynamics in the formulation of the constitutive relations, they do not consider thermo-mechanical coupling. This has been treated in two recent papers by

Chadwick and Powdrill⁹⁹ for the linear thermoelastic case and by Fine¹⁰⁰ for the thermoelastoplastic case.

In the hydrodynamic formulation of the shock wave problem, the major physical effect considered in the constitutive equation is compressibility, i.e., dilatational (volumetric) waves. Thus, shear waves, in fact any shear effects whatsoever, are not considered at all. As has been pointed out by Fyfe et al,¹⁰¹ this does not mean that the hydrodynamic theory cannot predict some physical aspects of a shock wave even at high velocities (as opposed to hypervelocities). An example of an early attempt to combine shear effects with dilatational effects is contained in Ref. 102.

It should be pointed out that shock waves are not limited to compressible media. In fact, recent analyses by Chu¹⁰³⁻¹⁰⁴ and by Collins¹⁰⁵ have been concerned with the propagation of shock waves in incompressible isotropic elastic media.* In such media, only nondilatational shock waves can occur.

Recently Bland,¹⁰⁶⁻¹⁰⁷ Green,⁸⁴ and Coleman, Gurtin, and Herrera,⁸⁸ considered plane shock waves in compressible isotropic elastic media. Although these investigators considered certain thermodynamic aspects, they did not consider them to the depth considered by Dewey¹⁰⁸ and by Lee and Wierzbicki.¹⁵ The case of plane shock waves in compressible isotropic thermoelastic media was recently treated by Chadwick and Powdrill.¹⁰⁹ Their analysis is interesting in that they claim that their analysis leads to an infinite family of shock wave solutions which range thermodynamically from isothermal to adiabatic. They claim that they know of no thermodynamic or mechanical principle which enables selection of the "correct" solution, although they suggest the possibility of using the theory of nonlinear hyperbolic partial differential equations or the irreversibility principle of thermodynamics (second law). The present writers suggest that a stability investigation might be in order here, i.e., it is unlikely that all of the possible solutions are stable.

* For an isotropic linearly elastic solid, incompressibility requires that Poisson's ratio be equal to 1/2. This value is closely approached in certain rubber-type materials, but not in metallic materials.

In Ref. 106, Bland found that two kinds of shock waves, dilatational and nondilatational, are possible in a compressible isotropic elastic solid. However, it is interesting to note that he concluded that nondilatational shock waves cannot propagate into a compressible hyperelastic solid at rest in its reference state. To the present writers, this implies that nondilatational shock waves can occur only during unloading, since then the material, being already loaded, is not at its reference state. In Ref. 107, Bland showed that in many solids (including simple elastic materials), the only kind of shock waves which are stable and admissible thermodynamically are tensile dilatational shock waves (in contrast to compressive dilatational shock waves in fluids). Although plane compressive shock waves in elastoplastic media have been studied extensively, Bland claimed that they are possible only in media in which the stress-strain curve is concave upward in the plastic range.

To study the shock structure (i.e. the shape of the shock wave front), it is necessary to include viscous dissipative effects. Recently Bland¹¹⁰ has performed such an analysis for plane waves in a simple viscoelastic solid. He showed that all monotonic wave profiles ultimately adopt the same constant wave profile, and he calculated the profile width and the time formation of the profile.

In this brief review, a number of related special topics should at least be mentioned:

1. Disintegration or pulverization of material behind a shock front, applicable to certain soils.¹¹¹
2. Changes of phase such as melting¹¹² due to shock wave heating, shock-induced metallurgical transformations,¹¹³ and shock hardening of metals.¹¹⁴
3. Interactions between acoustic waves and shock waves,¹¹⁵ reflection and refraction of shock waves at free surfaces and interfaces, and spallation fracture criteria.^{116,117}
4. Experimental techniques for generating shock waves and measuring various characteristics of them.¹⁻³

II. COUPLED THERMOELASTICITY THEORY FOR A LINEAR SOLID WITH MICROSTRUCTURE

A. INTRODUCTION

The use of high-pressure dynamic loading techniques in studying the behavior of solids under strong shock loading has produced a very large body of experimental data in recent years.³ Most of the original experimental work was associated with very high pressures (three or more orders of magnitude above the ultimate strength of the material) at which it has been recognized that strength effects are not important. Thus, the theory^{*} developed to accompany this work was based on hydrodynamics of dense fluids. Later interest turned to hypervelocity impact of a small body on a massive body. This problem involved creation of craters of finite size and consequently involved high-pressure waves that must necessarily depend on the strength properties of the materials involved. The natural extension of hydrodynamic theory to this problem has been by the most expedient addition of special effects to existing computer codes (programs) and in correlation of simple phenomenological models with experimental results.

There is a well recognized need for an attack on the problem of propagation of high-pressure waves from a fundamental thermomechanical point of view.¹⁵ This effort is underway in several areas. The effort reported here is concerned with developing an applicable coupled thermoelastic theory that will take into consideration the microstructure of an elastic solid.

*The use of "theory" here is in its most general sense, since most of what has been done in the past is in the nature of computer solutions to very involved nonlinear flow problems and might properly be called computer experiments on mathematical simulations.

The coupled thermomechanical theory (thermal and mechanical effects coupled in energy and constitutive equations) is well established for the macroscopic description of solid media. The elastic case is due to Duhammel⁵ in 1837, the viscoelastic case to Biot⁴⁰ in 1955, and the viscoplastic case to Dillon³⁵ in 1963.

Experimental observation of such mechanical phenomena as size effects and crystal-lattice type wave dispersion effects has led to various micromechanical theories. Of these, perhaps the most notable is the couple-stress theory, which in addition to ordinary stresses (forces per unit area) also considers couples per unit area. This theory was originated by Voigt⁸ in 1887 and was considerably developed by the Cosserat brothers⁹ approximately sixty years ago. In the past ten years, this theory has been developed further by various investigators too numerous to mention here.

Mindlin¹⁰ noted that couple stresses are actually only the antisymmetric part of a more general tensor which he called the double stress tensor; thus, he originated a theory which he called linear elasticity with microstructure. He also pointed out that his theory is mathematically equivalent to a linearized version of Ericksen and Truesdell's theory of deformable directors.¹¹⁸ In the latter theory, the mechanical behavior of a body at a given point is assumed to depend upon not only the deformation of the point but also the deformation of an oriented "director" located at the point. If the director is assumed to be rigid, the equations reduce to those of the Voigt-Cosserat couple-stress theory.

Upon completion of the present work, the work of Green, Rivlin, and Naghdi¹¹⁹⁻¹²¹ came to the attention of the authors. In Refs. 119 and 121 they derived an energy equation for a simple multipolar material, but they did not deal with constitutive equations. In Ref. 120 they extended their previous work to include multipolar deformation fields. Their work differs from ours in that they started with an entirely different set of

hypotheses in their theory. We believe that our derivation on the basis of a microelement is more satisfactory from a physical viewpoint. Also, they did not include initial stresses nor anisotropic behavior in their constitutive equation.

In the work reported here, the usual material constitutive equations are replaced by equations derived for the specific case of shock wave loading. This is consistent with the current interest in constitutive equations that have been experimentally determined from plate slap and other strong shock wave techniques.

B. CONSERVATION OF ENERGY

Using Mindlin's expression¹⁰ for the kinetic energy density, the kinetic energy T of a macrovolume V can be rewritten as follows.

$$T = \frac{1}{2} \int_V \rho \dot{u}_j \dot{u}_j dV + \frac{1}{6} \int_V \rho' d_{lj}^2 \dot{\psi}_{lk} \dot{\psi}_{jk} dV \quad (3a)$$

$$\text{where} \quad \rho = \rho_M + \rho' \quad (3b)$$

$$d_{lj}^2 = d_p d_q \left(\delta_{p1} \delta_{q1} l_{l1} l_{j1} + \delta_{p2} \delta_{q2} l_{l2} l_{j2} + \delta_{p3} \delta_{q3} l_{l3} l_{j3} \right) \quad (3c)$$

where

- u_j = displacement components
- d_i = semilengths of edges of microelement
- ψ_{ij} = microdeformation
- ρ_M = mass of macromaterial per unit macrovolume
- ρ' = mass of micromaterial per unit macrovolume
- δ_{ij} = Kronecker delta
- l_{ij} = direction cosines of edges of microelement with respect to fixed spatial coordinates X'_1

and a dot denotes differentiation with respect to time. The first term on the right-hand side of Eq. (3a) is the classical kinetic energy expression and the second term represents the contribution of the microelement.

Mindlin's¹⁰ expression for the rate of work W done on the macrovolume V by the external forces (surface and body types) is equivalent to the form:

$$W = \int_A t_j \dot{u}_j dA + \int_V f_j \dot{u}_j dV + \int_A T_{jk} \dot{\psi}_{jk} dA + \int_V F_{jk} \dot{\psi}_{jk} dV \quad (4)$$

where

t_i = surface force per unit area

f_i = body force per unit macrovolume

T_{jk} = surface force doublet per unit area with moment arm normal to axis X_j and acting in the X_k direction

F_{jk} = body force doublet per unit volume with same subscript notation as for T_{jk}

A = area

The terms on the right-hand side represent the work done by the respective macro and micro surface and body forces.

The internal energy U^* contained in both macroelements and microelements can be expressed as

$$U^* = \int_V \rho_M \bar{U}_M dV + \int_V \rho' U' dV = \text{total energy} - \text{kinetic energy} \quad (5)$$

where U_M , U' are the internal energies per unit mass for the macroelement and microelement, respectively.

Considering a closed system consisting of both macroelements and microelements, thermal energy is transferred out of the system at the rate

$$\dot{Q} = \int_A q \, dA \quad (6)$$

where q is the outward heat flux. Conservation of mechanical energy requires

$$\dot{W} - \dot{Q} = \frac{d}{dt} (T + U^*) \quad (7)$$

The traction conditions at the boundary of the macroelement are:

$$t_j = n_i (\bar{\sigma}_{ij} + \hat{\sigma}_{ij}) \quad (8a)$$

$$T_{jk} = n_i (\bar{\mu}_{ijk} + \hat{\mu}_{ijk}) \quad (8b)$$

where n_i = direction cosines of the outer normal to the surface

$\bar{\sigma}_{ij}, \hat{\sigma}_{ij}$ = components of the respective symmetric and antisymmetric parts of the ordinary stress vector (force/area)

$\bar{\mu}_{ijk}, \hat{\mu}_{ijk}$ = components of the respective symmetric and antisymmetric parts of the doublet stress vector (force doublet/area) acting normal to direction X_i

Application of the divergence theorem and Eqs. (8) yields the following result from Eq. (4):

$$\begin{aligned} \dot{W} = & \int_V \left[(\bar{\sigma}_{ij} + \hat{\sigma}_{ij}) \dot{u}_j \right]_{,i} dV + \int_V \left[(\bar{\mu}_{ijk} + \hat{\mu}_{ijk}) \dot{\psi}_{jk} \right]_{,i} dV \\ & + \int_V \epsilon_{ij} \dot{u}_j dV + \int_V F_{jk} \dot{\psi}_{jk} dV \end{aligned} \quad (9)$$

where $[]_{,i} = \partial [] / \partial X_i$

The heat transfer can be rewritten in terms of a heat flux vector as follows:

$$Q = \int_A q_j n_j dA = \int_V q_{j,j} dV \quad (10)$$

The differentiation on the right-hand side of Eq. (5) can be brought under the integral signs appearing in Eqs. (1) and (3) with the following results:

$$\begin{aligned} \frac{d}{dt} (T + U^*) &= \int_V \rho \ddot{u}_j \dot{u}_j dV + \frac{1}{3} \int_V \rho' d_{\ell j}^2 \ddot{\psi}_{\ell k} \dot{\psi}_{jk} dV \\ &+ \int_V (\rho_M \dot{U}_M + \rho' \dot{U}') dV \end{aligned} \quad (11)$$

This interchange of the order of differentiation and integration can be justified by assuming small displacements.⁶ However, it can also be justified for arbitrary displacements by considering conservation of mass.¹²² Consistent with the assumptions of linear elastodynamics the densities are treated as constants.

The quantity $\dot{u}_{j,i}$ may be written in terms of its symmetric and antisymmetric parts as follows:

$$\dot{u}_{j,i} = \frac{1}{2} (\dot{u}_{i,j} + \dot{u}_{j,i}) - \frac{1}{2} (\dot{u}_{i,j} - \dot{u}_{j,i}) = \dot{\epsilon}_{ij} - \dot{\omega}_{ij} \quad (12a)$$

where ϵ_{ij} and ω_{ij} are the macrostrain and macrorotation, respectively, given by the following relations:

$$\epsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}), \quad \omega_{ij} = \frac{1}{2} (u_{i,j} - u_{j,i}) \quad (12b)$$

The relative deformation γ_{ij} is defined as the difference between the macrodisplacement gradient and the microdeformation, i.e.

$$\gamma_{ij} = u_{j,i} - \psi_{ij} \quad (13a)$$

From Eqs. (10a) and (11), the following relationship is obtained:

$$u_{j,i} = \epsilon_{ij} - \omega_{ij} = \psi_{ij} + \gamma_{ij} \quad (13b)$$

Then the first term in the expression for W , Eq. (7), can be rewritten as follows:

$$\int_V \left[(\bar{\sigma}_{ij,i} + \hat{\sigma}_{ij,i}) \dot{u}_j + \bar{\sigma}_{ij} \dot{\epsilon}_{ij} + \hat{\sigma}_{ij} (\dot{\psi}_{ij} + \dot{\gamma}_{ij}) \right] dV \quad (14)$$

where the integrand term $-\bar{\sigma}_{ij} \dot{\omega}_{ij}$ has been omitted because it is a product (of a symmetric tensor and an antisymmetric tensor) which must be zero.

Incorporating relations (9-11, 12) into (7) and rearranging terms and subscripts yields:

$$\begin{aligned} & \int_V (\bar{\sigma}_{ij,i} + \hat{\sigma}_{ij,i} + f_j - \rho \ddot{u}_j) \dot{u}_j dV \\ & + \int_V \left[\bar{\mu}_{ijk,i} + \hat{\mu}_{ijk,i} + \hat{\sigma}_{jk} + F_{jk} - \frac{1}{3} \rho' d_{\ell j}^2 \ddot{\psi}_{k\ell} \right] \dot{\psi}_{jk} dV \\ & + \int_V \left[\bar{\sigma}_{ij} \dot{\epsilon}_{ij} + \hat{\sigma}_{jk} \dot{\gamma}_{jk} + (\bar{\mu}_{ijk} + \hat{\mu}_{ijk}) \dot{\psi}_{jk,i} - q_{j,j} - \rho_M \dot{U}_M - \rho' \dot{U}' \right] dV = 0 \end{aligned} \quad (15)$$

The first two integrals appearing in Eq. (15) vanish by virtue of the following translational and rotational equations of motion:

$$\bar{\sigma}_{ij,i} + \hat{\sigma}_{ij,i} + f_j = \rho \ddot{u}_j \quad (16)$$

$$\bar{\mu}_{ijk,i} + \hat{\mu}_{ijk,i} + \hat{\sigma}_{jk} + F_{jk} = \frac{1}{3} \rho' d_{kl}^2 \ddot{\psi}_{kl} \quad (17)$$

Thus, the only integral remaining in Eq. (15) is the last one, which then must be equal to the right-hand side, namely zero. Furthermore, for this integral to be zero for arbitrarily small regions, its integrand must be zero. Thus,

$$\bar{\sigma}_{ij} \dot{\epsilon}_{ij} + \hat{\sigma}_{jk} \dot{\gamma}_{jk} + (\bar{\mu}_{ijk} + \hat{\mu}_{ijk}) \dot{\psi}_{jk,i} - q_{j,j} = \rho \dot{U} \quad (18)$$

where

$$\rho U = {}_M U_M + \rho' U'$$

The microstrain gradient κ_{ijk} is defined as follows:

$$\kappa_{ijk} = \psi_{jk,i} \quad (19)$$

Then Eq. (18) can be rewritten in the following form:

$$\bar{\sigma}_{ij} \dot{\epsilon}_{ij} + \hat{\sigma}_{jk} \dot{\gamma}_{jk} + \bar{\mu}_{ijk} \dot{\kappa}_{ijk} + \hat{\mu}_{ijk} \dot{\kappa}_{ijk} - q_{j,j} = \rho \dot{U} \quad (20)$$

Equation (18) is the general energy equation for an elastic medium with microstructure. When microstructural effects are absent ($\bar{\mu}_{ijk} = \hat{\mu}_{ijk} = \psi_{kl} \equiv 0$), Eq. (17) requires that the antisymmetric part of the ordinary stress tensor also vanish ($\hat{\sigma}_{jk} \equiv 0$) and Eq. (20) reduces to the well-known energy equation of a classical elastic solid.⁵

It is of interest to note that when all of the stress (σ and μ), strain (ϵ, γ) and strain gradient (κ) components have the same sign, the presence of the antisymmetric ordinary stresses and both the symmetric and antisymmetric parts of the doublet stresses represent energy sinks in the system.

It is especially important to note that even though Eq. (20) is coupled in the sense that it involves terms containing σ_{ij} , μ_{ijk} , $\dot{\gamma}$, and U , there are no cross-energy terms such as $\hat{\sigma}_{ij}\hat{\kappa}_{ijk}$ or $\hat{\mu}_{ijk}\dot{\epsilon}_{ij}$. This considerably reduces the number of coefficients which are required in the constitutive equations.

C. DERIVATION OF CONSTITUTIVE EQUATIONS

Using Caratheodory's statement of the second law of thermodynamics, Boley and Weiner⁶ derived the following relations for a locally reversible thermodynamic process:*

$$A_s \dot{\alpha}_s + \rho T \dot{\eta} = \dot{U} \quad (21a)$$

$$B_t \dot{\beta}_t - q_{j,j} = \rho T \dot{\eta} \quad (21b)$$

where α_s, β_t = nondissipative and dissipative deformation variables

A_s, B_t = state functions

ρ = density

T = absolute temperature

η = entropy density function

Here we neglect viscous effects because it is believed that shock wave deformation occurs so rapidly that there is insufficient time for viscous forces to develop; thus, $B_t \dot{\beta}_t = 0$. Then Eq. (21b) yields:

$$q_{j,j} = -\rho T \dot{\eta} \quad (22)$$

* According to Coleman and Mizel¹²³ the assumption of microscopic reversibility is unnecessary.

Taking ϵ_{ij} , γ_{jk} , κ_{ijk} as state variables, we must consider $\bar{\sigma}_{ij}$, $\hat{\sigma}_{jk}$, μ_{ijk} as state functions:

$$\begin{aligned}\bar{\sigma}_{ij} &= \bar{\sigma}_{ij}(\epsilon_{ij}, \gamma_{jk}, \kappa_{ijk}, T) \\ \hat{\sigma}_{jk} &= \hat{\sigma}_{jk}(\epsilon_{ij}, \gamma_{jk}, \kappa_{ijk}, T)\end{aligned}\quad (23)$$

$$\mu_{ijk} = \mu_{ijk}(\epsilon_{ij}, \gamma_{jk}, \kappa_{ijk}, T)$$

$$\bar{\sigma}_{ij}\dot{\epsilon}_{ij} + \hat{\sigma}_{jk}\dot{\gamma}_{jk} + \mu_{ijk}\dot{\kappa}_{ijk} + pT\dot{\eta} = \rho\dot{U}$$

A free-energy function ϕ is defined by the following equation:

$$\phi(\epsilon_{ij}, \gamma_{jk}, \kappa_{ijk}, T) = U(\epsilon_{ij}, \gamma_{jk}, \kappa_{ijk}, T) - T\eta(\epsilon_{ij}, \gamma_{jk}, T)\quad (24)$$

Then

$$\dot{\phi} = \dot{U} - T\dot{\eta} - \dot{T}\eta\quad (25)$$

But since

$$\begin{aligned}\phi &= \phi(\epsilon_{ij}, \gamma_{jk}, \kappa_{ijk}, T) \\ \dot{\phi} &= \frac{\partial \phi}{\partial \epsilon_{ij}} \dot{\epsilon}_{ij} + \frac{\partial \phi}{\partial \gamma_{jk}} \dot{\gamma}_{jk} + \frac{\partial \phi}{\partial \kappa_{ijk}} \dot{\kappa}_{ijk} + \frac{\partial \phi}{\partial T} \dot{T}\end{aligned}\quad (26)$$

Equating from Eqs. (25) and (26):

$$\dot{U} - T\dot{\eta} - \dot{T}\eta = \frac{\partial \phi}{\partial \epsilon_{ij}} \dot{\epsilon}_{ij} + \frac{\partial \phi}{\partial \gamma_{jk}} \dot{\gamma}_{jk} + \frac{\partial \phi}{\partial \kappa_{ijk}} \dot{\kappa}_{ijk} + \frac{\partial \phi}{\partial T} \dot{T}\quad (27)$$

Thus, since it has been assumed that the other quantities are independent of \dot{T} , comparison of Eqs. (26) and (27) shows that

$$\eta = - \frac{\partial \phi}{\partial T}\quad (28)$$

and

$$\dot{U} = \dot{n}T + \frac{\partial \phi}{\partial \epsilon_{ij}} \dot{\epsilon}_{ij} + \frac{\partial \phi}{\partial \gamma_{jk}} \dot{\gamma}_{jk} + \frac{\partial \phi}{\partial \kappa_{ijk}} \dot{\kappa}_{ijk} \quad (29)$$

Putting Eq. (29) into Eq. (23) gives

$$\bar{\sigma}_{ij} \dot{\epsilon}_{ij} + \hat{\sigma}_{jk} \dot{\gamma}_{jk} + \mu_{ijk} \dot{\kappa}_{ijk} = \rho \left(\frac{\partial \phi}{\partial \epsilon_{ij}} \dot{\epsilon}_{ij} + \frac{\partial \phi}{\partial \gamma_{jk}} \dot{\gamma}_{jk} + \frac{\partial \phi}{\partial \kappa_{ijk}} \dot{\kappa}_{ijk} \right) \quad (30)$$

Since it has been assumed that ϕ is independent of $\dot{\epsilon}_{ij}$, $\dot{\gamma}_{ij}$, and $\dot{\kappa}_{ijk}$, the following additional equations must be satisfied:

$$\bar{\sigma}_{ij} = \rho \frac{\partial \phi}{\partial \epsilon_{ij}}, \quad \hat{\sigma}_{jk} = \rho \frac{\partial \phi}{\partial \gamma_{jk}}, \quad \mu_{ijk} = \rho \frac{\partial \phi}{\partial \kappa_{ijk}} \quad (31a) \quad (31b) \quad (31c)$$

Equation (31a) has often been used as the thermodynamic basis for the symmetry of the elastic coefficients in the generalized Hooke's law for a general anisotropic elastic solid. In analogous fashion, Eq. (31b) can now be used to establish the symmetry of the microstructural elastic coefficients in general (anisotropic). It is of fundamental importance to note that Eqs. (31) show that thermodynamically there can be no coupling of macrostrains and microstrains in the constitutive equations. Needless to say, this simplifies the constitutive equations considerably.

To establish the form of the macro and micro constitutive equations more specifically, the free-energy function can be assumed to be a polynomial in the macrostrain components ϵ_{ij} , the relative strain components γ_{ij} , the macrostrain-gradient components κ_{ijk} , and the temperature T . For a linear material, defined as one having linear constitutive relations, the highest degree polynomial required is of second degree. Thus,

$$\begin{aligned} \rho \phi = & a + b_{ij} \epsilon_{ij} + d_{ijkl} \epsilon_{ij} \epsilon_{kl} + g_{ij} \epsilon_{ij} T \\ & + b_{jk}^* \gamma_{jk} + d_{jk}^* \gamma_{jk} \gamma_m + g_{jk}^* \gamma_{jk} T \\ & + B_{ijl} \kappa_{ijl} + D_{ijk\ell mn} \kappa_{ijk} \kappa_{\ell mn} + G_{ijk} \kappa_{ijk} T \end{aligned} \quad (32)$$

In view of Eqs. (31) and (32), the following constitutive equations can be written:

$$\bar{\sigma}_{ij} = b_{ij} + d_{ijij}\epsilon_{ij} + d_{ijkl}\epsilon_{kl} + g_{ij}T; kl \neq ij \quad (33)$$

$$\hat{\sigma}_{ij} = b_{jk}^* + d_{jkjk}^*\gamma_{jk} + d_{jk\ell m}^*\gamma_{\ell m} + g_{jk}^*T; \ell m \neq jk \quad (34)$$

$$\mu_{ijk} = B_{ijk} + D_{ijkijk}\kappa_{ijk} + D_{ijk\ell mn}\kappa_{\ell mn} + G_{ijk}T; \ell mn \neq ijk \quad (35)$$

There is a total of forty independent parameters involved in a general three-dimensional thermoelastic problem involving microstructure. These are temperature plus thirty-nine mechanical deformation parameters:

Six	ϵ_{ij}	(since $\epsilon_{ji} = \epsilon_{ij}$)
Six	γ_{jk}	(since $\gamma_{kj} = -\gamma_{jk}$)
Twenty-seven	κ_{ijk}	

(Mindlin⁸ stated that there are forty-two mechanical deformation parameters, but he had not determined that $\gamma_{kj} = -\gamma_{jk}$.)

The arrays of coefficients have the following sizes:

Coefficient Array	Type (a)	Total No. of Non-Zero Coefficients	No. of Independent Coefficients
b	IM	6	6
d	AM	36	21
g	T	3(b)	3(b)
b*	IM	6	3
d*	AM	36	15
g*	T	6	3
B	IM	27	27
D	AM	729	729
G	T	27	27
	Total IM	39	36
	Total AM	801	765
	Total T	36	33
	Grand Total	876	834

(a) IM = initial mechanical, AM = active mechanical, T = thermal expansion

(b) This relies on the well-established fact that there are no thermal shear strains in linear theory.

The total number of independent active mechanical coefficients listed in the above tabulation (765) is considerably smaller than the 1764 claimed by Mindlin,¹⁰ although it is still a formidable number. The advantage of including anisotropic behavior both on a macroscopic and on a microscopic scale is that it permits handling of any material. However, many metals and alloys of engineering importance (steel, aluminum, some titanium) are macroscopically isotropic and microscopically anisotropic depending upon the crystalline structure.

Recently Gurtin^{124,125} proved a theorem stating that the Clausius-Duhem inequality requires that every elastic material be "simple," i.e., have stress, free energy, and entropy at a material point dependent at most on deformation gradient and temperature at that point. However, Gurtin did not include the possibility of any doublet stress effects in his work. Thus, the present work is not inconsistent with his theorem; rather it is beyond the scope of his theorem.

D. RELATION TO OTHER THEORIES

It may be possible to relate the present theory to the solid-state theory of the Grüneisen parameter.¹²⁶⁻¹²⁸ For example, Gilgarry¹²⁸ has argued that the Dugdale-MacDonald corrections¹²⁷ for finite strain are not valid; yet many experiments indicate better agreement with the Dugdale-MacDonald predictions.

It has been shown that there is a direct correspondence between doublet stresses and a continuous distribution of dislocations.^{129,130} This may provide a basis for relating the present work to various theories of dislocational damping.^{131,132}

The present theory has no provisions for phase and state transformations, which sometimes take place in certain crystalline materials under strong shock conditions.³

III. DILATION WAVES INCLUDING THE EFFECTS OF MICROSTRUCTURE

A. INTRODUCTION

The accumulation of a number of years of experimental work with shock waves in solids is reported in Ref. 133. That work has led to the conclusion that any proper explanation of shock wave phenomena in solids must include the effects of a rotation and deformation of microscopic regions even when the input loading is a longitudinal pulse. These conclusions provide sufficient reason for the investigation of a theory of "microstructural" deformation in shock wave processes. A necessary requirement for such an investigation is the development of appropriate constitutive equations as done above.

These constitutive equations are used here with the equations of motion for plane waves.

B. DEFINITION OF AN IDEAL ELASTIC SOLID WITH MICROSTRUCTURE FOR SHOCK WAVE STUDIES

The definition of an "ideal" continuum involves the assumption that a state variable (vector) exists and that a reversible path exists between any two possible conditions of the state vector. The state vector for an ideal elastic solid with microstructure must include the temperature, T , and information about either the state of stress or strain in both conventional macrostructure and the additional microstructure. Constitutive equations have been developed which involve the state variables ϵ_{ij} , γ_{jk} , and κ_{ijk} (macrostrain, relative deformation between macro and micro media, and the microstrain gradient), and the state functions:

$$\bar{\sigma}_{ij}(\epsilon_{ij}, \gamma_{jk}, \kappa_{ijk}, T) = \text{symmetric macrostress} \quad (36)$$

$$\hat{\sigma}_{ik}(\epsilon_{ij}, \gamma_{jk}, \kappa_{ijk}, T) = \text{unsymmetric macrostress} \quad (37)$$

and

$$\nu_{ijk}(\epsilon_{ij}, \gamma_{jk}, \kappa_{ijk}, T) = \text{doublet stress.} \quad (38)$$

This development is valid whenever the kinematics of the physical problem make Eulerian and Lagrangian coordinates interchangeable. In particular, the assumption is made that

$$\frac{\partial u_j}{\partial a_i} \approx \frac{\partial u_j}{\partial x_i} \quad (39)$$

where $u_j = x_j - a_j$ is the displacement of the particle, x_j is the Eulerian coordinate and a_j is the Lagrangian coordinate. And a similar assumption applies to derivatives in the microstructure. In the problems where the absolute value of displacement gradients is small, i.e., where

$$\left| \frac{\partial u_j}{\partial a_i} \right| \ll 1 \quad (40)$$

this is a valid approximation. However, we wish to deal with shock waves in the macrostructure where this approximation could be considered invalid. The validity of the assumption in reference to the microstructure also needs to be considered. The size of the microstructure elements has been related to the spacing of dislocations in Ref. 133. In Ref. 134, a typical value for the density of dislocations in a crystalline structure is suggested as $10^9/\text{cm}^2$ before shock wave loading and $10^{11}/\text{cm}^2$ after loading.

This would lead to typical cell sizes of $3 \cdot 10^{-5}$ cm/cell edge before and $3 \cdot 10^{-6}$ cm/cell edge after shock wave loading. The same reference also suggests that the shock front thickness would typically be of the order of a phonon mean free path or from 10^{-5} cm to 10^{-7} cm, which is comparable to the cell size. This leaves the speculation that the gradient is not small in the microstructure with some support. Consequently it will be necessary to reexamine the formulation of the microstructural representation.

The Eulerian equations of motion for an elastic solid with microstructure are¹⁰

$$\frac{\partial}{\partial x_i} (\bar{\sigma}_{ij} + \hat{\sigma}_{ij}) + \rho f_j = \rho \ddot{u}_j \quad (41a)$$

$$\frac{\partial}{\partial x_i} (\bar{\mu}_{ijk} + \hat{\mu}_{ijk}) + \hat{\sigma}_{jk} + \rho F_{jk} = \frac{1}{3} \rho' d_{kl}^2 \ddot{\psi}_{kl} \quad (41b)$$

These equations are converted to Lagrangian form by substitution of the Lagrangian variables.

$$\frac{\partial}{\partial a_i} \left(\bar{\sigma}_{ij}^{(L)} \right) + \hat{\sigma}_{ij}^{(L)} + \rho_o f_j^{(L)} = \rho_o \ddot{u}_j \quad (42a)$$

$$\frac{\partial}{\partial a_i} \left(\bar{\mu}_{ijk}^{(L)} \right) + \hat{\mu}_{ijk}^{(L)} + \hat{\sigma}_{jk}^{(L)} + \rho' F_{jk}^{(L)} = \frac{1}{3} \rho' (d_{kl}^{(L)})^2 \ddot{\psi}_{kl} \quad (42b)$$

The Eulerian symmetric stress tensor σ_{ij} gives rise to a non-symmetric Lagrangian stress tensor $\sigma_{ij}^{(L)}$. In order to recapture a symmetric stress tensor, the Lagrangian tensor may be transformed to the Kirchhoff stress tensor, and Eq. (7a) becomes

$$\frac{\partial}{\partial a_i} \left[\left(\bar{\sigma}_{ik}^{(K)} + \hat{\sigma}_{ik}^{(K)} \right) \frac{\partial x_j}{\partial a_k} \right] + \rho_o f_j^{(L)} = \rho_o \ddot{u}_j$$

In order to simplify the notation, we let $f_j^{(L)} \equiv f_j$ and define

$$\sigma^{(K)} = S$$

so that the macro material equation of motion in Lagrangian coordinates becomes

$$\frac{\partial}{\partial a_i} \left[(\bar{S}_{ik} + \hat{S}_{ik}) \frac{\partial x_j}{\partial a_k} \right] + \rho_o f_j = \rho_o \ddot{u}_j \quad (43a)$$

Use may be made of the definition of μ_{ijk} as a gradient of the scalar potential energy of an elastic solid¹⁰ to obtain an equivalent "Kirchhoff" doublet stress in the following form

$$\mu_{ijk}^{(K)} = \left(\frac{\rho_0}{\rho} \right) \frac{\partial a'_i}{\partial x'_\delta} \frac{\partial a'_j}{\partial x'_\delta} \frac{\partial a'_k}{\partial x'_\epsilon} \mu_{\gamma\delta\epsilon}$$

While the relation between the "Kirchhoff" and "Lagrangian" forms of the doublet stress is

$$\mu_{ilm}^{(K)} \frac{\partial x'_l}{\partial a'_j} \frac{\partial x'_m}{\partial a'_k} = \mu_{ijk}^{(L)}$$

The desired form of the micro material equation of motion is obtained as

$$\frac{\partial}{\partial a_i} \left[\left(\bar{M}_{ilm} + \hat{M}_{ilm} \right) \frac{\partial x'_j}{\partial a'_l} \frac{\partial x'_k}{\partial a'_m} \right] + \hat{S}_{jk} \frac{\partial x_j}{\partial a_k} + \rho_0 F_{jk} = \frac{1}{3} \rho'_0 (d_{kl})^2 \ddot{\psi}_{kl} \quad (43b)$$

with the simplifying notation $\mu^{(K)} = M$, $d^{(L)} = d$ and $F_{jk}^{(L)} \equiv F_{jk}$

Equations (43a) and (43b) are the equations of motion for use with plane wave phenomena.

C. PLANAR WAVE IN MICROMEDIA

In a macromedia the planar wave is defined by requiring all spacial derivatives to be zero except for those in the direction of the wave propagation, i.e. $\frac{\partial}{\partial a_1} () \neq 0$, $\frac{\partial}{\partial a_i} () = 0$, $i = 2, 3$. The same idea may be extended to the micromedia, in which case $\frac{\partial}{\partial a_1} () \neq 0$, $\frac{\partial}{\partial a_i} () = 0$, $i = 2, 3$. When this is done, Eqs. (43a) and (43b) take the form

$$\frac{\partial}{\partial a} \left[(\bar{S} + \hat{S}) \frac{\partial x}{\partial a} \right] + \rho_0 f = \rho_0 \ddot{u} \quad (44a)$$

$$\frac{\partial}{\partial a} \left[M \left(\frac{\partial x}{\partial a} \right)^2 \right] + \hat{S} \frac{\partial x}{\partial a} + \rho_0 F = \frac{\rho_0 d^2}{3} \ddot{\psi} \quad (44b)$$

If we introduce the notion that $\partial u / \partial a$ is a measure of the wave strength¹⁰⁷ (or shock strength), then we may give a meaning to $\partial x / \partial a$ in the following way: Let $\lambda = \partial u / \partial a$ and recall that $u = x - a$, so that $\frac{\partial x}{\partial a} = 1 + \lambda$, then Eqs. (44a) and (44b) become (for $f = F = 0$)

$$\frac{\partial}{\partial a} [(\bar{S} + \hat{S})(1 + \lambda)] = \rho_o \ddot{u} \quad (45a)$$

$$(1 + \lambda)\hat{S} = \frac{\rho_o d^2}{3} \ddot{\psi} - \frac{\partial}{\partial a} [M(1 + \psi)^2] \quad (45b)$$

Again following Bland,¹⁰⁷ the stresses are replaced by derivatives of the potential energy function, which we will call W . So that^{*}

$$\bar{S} = \frac{\partial W}{\partial \epsilon} \left(\text{and } \epsilon = \lambda + \frac{1}{2} \lambda^2 \right)$$

$$M = \frac{\partial W}{\partial \kappa}$$

In addition, note that

$$\frac{\partial W}{\partial \lambda} = \frac{\partial W}{\partial \epsilon} \frac{\partial \epsilon}{\partial \lambda} = \frac{\partial W}{\partial \epsilon} (1 + \lambda)$$

and

$$\frac{\partial}{\partial a} \left(\frac{\partial W}{\partial \lambda} \right) = \frac{\partial^2 W}{\partial \lambda^2} \frac{\partial \lambda}{\partial a} = \frac{\partial^2 W}{\partial \lambda^2} \frac{\partial^2 u}{\partial a^2}$$

then Eq. (10a) becomes

$$\frac{\partial^2 W}{\partial \lambda^2} \cdot \frac{\partial^2 u}{\partial a^2} + \frac{\partial}{\partial a} [(1 + \lambda)\hat{S}] = \rho_o \ddot{u} \quad (46a)$$

In order to make a similar elimination of M , one needs to differentiate the last term in Eq. (45b).

^{*}For the present we will not alter \hat{S} .

Equation (45b) with M replaced by $\frac{\partial W}{\partial \kappa}$ and carrying out the differentiation gives

$$(1 + \lambda)\hat{s} = \frac{\rho_0 d^2}{3} \ddot{\Psi} - \left[(1 + \psi)^2 \frac{\partial^2 W}{\partial \kappa^2} \frac{\partial \kappa}{\partial a} + \frac{\partial W}{\partial \kappa^2} (1 + \psi) \frac{\partial \Psi}{\partial a} \right]$$

But

$$\kappa = \frac{\partial \Psi}{\partial a}$$

so that

$$\frac{\partial \kappa}{\partial a} = \frac{\partial^2 \Psi}{\partial a^2}$$

Then

$$(1 + \lambda)\hat{s} = \frac{\rho_0 d^2}{3} \ddot{\Psi} - \frac{\partial^2 W}{\partial \kappa^2} \frac{\partial^2 \Psi}{\partial a^2} - \left[(2 + \psi) \psi \frac{\partial^2 \Psi}{\partial a^2} \frac{\partial^2 W}{\partial \kappa^2} + 2\psi \frac{\partial \Psi}{\partial a} \frac{\partial W}{\partial \kappa} \right] \quad (46b)$$

It is clear that if Eq. (46b) is introduced into Eq. (46a) a very complicated partial differential equation results. In order to find any acceptable simplification of these equations, we wish to know what physical facts can be used to simplify the mathematics of the problem at this point?

Up to the end of the elastic regime, the wave equation (obtained by $\hat{s} = 0$ in Eq. (46a)) gives a very good approximation to the experimental observations. This seems to be true even when a large number of dislocations are present (i.e., when a microstructure is present).

We will appeal to these observations as an argument for setting $\hat{s} = 0$ and see if its consequence gives any meaningful results. To do this we must study the simultaneous equations:

$$\rho_o \ddot{u} - \frac{\partial^2 W}{\partial \lambda^2} \frac{\partial^2 u}{\partial c^2} = 0 \quad (47a)$$

$$\frac{\rho_o d^2}{3} \ddot{\psi} - \frac{\partial^2 W}{\partial \kappa^2} \frac{\partial^2 \psi}{\partial a^2} - 2 \frac{\partial W}{\partial \kappa} \frac{\partial \psi}{\partial a} = (2 + \psi) \psi \frac{\partial^2 \psi}{\partial a^2} \frac{\partial^2 W}{\partial \kappa^2} + 2 \psi \frac{\partial \psi}{\partial a} \frac{\partial W}{\partial \kappa} \quad (47b)$$

and the constitutive equation

$$W = A + B\lambda + C\lambda^2 + D\lambda T + F\kappa + G\kappa^2 + H\kappa T \quad (47c)^*$$

with proper boundary and initial conditions. For now we take $D = H = A = 0$. Then the behavior of Eq. (47a) is well known and Eq. (47b) becomes the equation of interest. Substituting W into Eq. (47b) leads to:

$$\begin{aligned} \frac{\rho_o d^2}{3} \ddot{\psi} - 2G \frac{\partial^2 \psi}{\partial a^2} - 2(F) \frac{\partial \psi}{\partial a} &= 2G \left(\frac{\partial \psi}{\partial a} \right) \\ &+ 2(2 + \psi) \psi \frac{\partial^2 \psi}{\partial a^2} G + 2\psi \frac{\partial \psi}{\partial a} \left(F + 2G \frac{\partial \psi}{\partial a} \right) \end{aligned} \quad (48a)$$

The right hand of Eq. (48a) is highly nonlinear. In order to see if anything can be done simply, we will arbitrarily set all nonlinear terms to zero (the validity of this step must be evaluated). So doing gives Eq. (48b)

$$\frac{\rho_o d^2}{3} \ddot{\psi} - 2G \frac{\partial^2 \psi}{\partial a^2} - 2F \frac{\partial \psi}{\partial a} = 0 \quad (48b)$$

* Equation (32).

In order to make the study of Eq. (48b) easier, nondimensional variables are introduced in the form:

$$\psi = \frac{1}{2} \frac{G^2}{F} \phi$$

$$a = \frac{G}{F} \zeta$$

$$\tau = \frac{d}{F} \sqrt{\frac{G\rho_o}{6}} \tau$$

with the result

$$\phi_{\zeta\zeta} - \phi_{\tau\tau} - \phi_{\tau} = 0 \quad (49)$$

Equation (49) has the form of the telegraph equation with space and time variables having their roles transposed. A substitution of the form $\phi = \phi e^{-\zeta/2}$ transforms Eq. (49) into

$$\phi_{\zeta\zeta} = \phi_{\tau\tau} + \frac{1}{4} \phi \quad (50)$$

and a formal solution with initial conditions of $\phi_{\zeta}(\zeta, 0) = P(\zeta)$, $\phi(\zeta, 0) = 0$ yields

$$\phi(\zeta, \tau) = e^{-\zeta/2} \int_0^{\zeta} J_0 \left(\frac{1}{2} \sqrt{\zeta^2 - \rho^2} \right) Q(\rho, 0) d\rho \quad (51a)$$

where

$$Q(\rho, \tau) = \frac{1}{2} [P(\rho + \tau) + P(\rho - \tau)] \quad (51b)$$

But $P(\rho + \tau)$ corresponds to $\tau < 0$ and does not exist. And since the initial velocity $P(\zeta)$ is applied only at the surface $\zeta = 0$, it can be represented as a delta function $P(\zeta) = \delta(\zeta)$ so that Eqs. (51) give

$$\phi(\zeta, \tau) = e^{-\zeta/2} \frac{1}{2} \int_0^{\zeta} J_0 \left(\frac{1}{2} \sqrt{\zeta^2 - \rho^2} \right) \delta(\rho - \tau) d\rho \quad (52)$$

The solution for $\tau \geq \zeta \geq 0$ is

$$\phi(\zeta, \tau) = \frac{1}{2} e^{-\zeta/2} J_0 \left(\frac{1}{2} \sqrt{\tau^2 - \zeta^2} \right) \quad (53)$$

and for $\tau < \zeta$ the signal has not yet arrived at ζ , so $\phi = 0$. Returning Eq. (53) to dimensional notation yields

$$\frac{\partial u'}{\partial a'} = \frac{1}{2} \frac{G^2}{F} e^{-F/2G a'} J_0 \left(\frac{1}{2} \sqrt{\frac{6F^2}{G\rho_o d^2} t'^2 - \frac{F^2}{G^2} a'^2} \right) \quad (54)$$

for an initial microstrain velocity

$$\frac{\partial}{\partial t} \frac{\partial u'}{\partial a'} = \sqrt{\frac{3G^3}{2\rho_o}} \frac{1}{Fd} \quad (55)$$

corresponding to $\phi_\tau = 1$.

This result corresponds to an oscillating decay of microstrain as a function of position along the space axis.

If $F = 0$ in the constitutive equation (Eq. (47c)), then Eq. (48b) becomes

$$\frac{\rho_o d^2}{3} \ddot{\psi} - 2G \frac{\partial^2 \psi}{\partial a^2} = 0$$

This is a standard wave equation and the microstrain may take any form that is a solution to a wave equation. Now if either of these cases obtains, then a space oscillation of microstrain is a possible elastic solution. Since there has been experimental evidence of a space oscillation in strain hardness after shock loading,¹³³ it is tempting to speculate on whether or not these oscillating solutions can be related

to the strain hardness observations. If the loading takes place so rapidly that the deformation extends its elastic range on loading, there may be some correlation between these results and those for which oscillation of the strain hardening has been observed.

APPENDIX

THERMODYNAMICALLY VALID THERMOELASTIC CONSTITUTIVE RELATIONS CONSIDERING TEMPERATURE DEPENDENCY OF THE ELASTIC COEFFICIENTS AND STRESS DEPENDENCY OF THE THERMAL-EXPANSION COEFFICIENT

There are two ways to formulate the thermodynamics of solids. Traditionally, it has been assumed that deformation gradients (strains) and temperature are the thermodynamic fluxes (i.e., the independent variables, also called state variables), while stress was considered as the thermodynamic force (i.e., the dependent variable, also called the state function). However, in some instances^{19,135} stress and temperature were considered as the independent variables and strain as the dependent variable. In his recent paper on thermodynamics of strained solids, Kestin²⁷ stated explicitly that either strain or stress could be used as the independent variable. The latter formulation is believed to be more desirable for the following reasons:

1. Prestress (i.e., initial stress) is included in a much more natural fashion, as discussed by Burridge and Knopoff.²⁰ Prestress must be considered in problems involving unloading waves.
2. The definitions of the elastic and thermal-expansion coefficients permit a much simpler derivation of the interrelationship between temperature dependency of the elastic coefficients and stress dependency of the thermal-expansion coefficient.
3. As shown by Westergaard, it is easier to deal with nonlinear stress-strain relations by complementary energy as a function of stress rather than strain energy as a function of strain.
4. The yield criterion (or plastic potential) in plasticity theory is a function of stress not strain.

In view of these considerations, especially the second one, the formulation having stress and temperature as the independent variables will be used here.

The energy equation is as follows:

$$\epsilon_{ij} \dot{\sigma}_{ij} + T \dot{\eta} = \dot{U} \quad (A1)$$

where ϵ_{ij} is the strain tensor, σ_{ij} is the stress tensor, T is absolute temperature, η is the entropy per unit-reference-state volume,^{*} U is the internal energy per unit-reference-state volume,^{*} and a dot denotes a derivative with respect to time.

The free-energy function is now defined as follows:

$$\phi(\sigma_{ij}, T) = U(\sigma_{ij}, T) - T\eta(\sigma_{ij}, T) \quad (A2)$$

Putting Eq. (A2) into Eq. (A1) gives

$$(\epsilon_{ij} - \partial\phi/\partial\sigma_{ij}) \dot{\sigma}_{ij} - (\eta + \partial\phi/\partial T) \dot{T} = 0 \quad (A3)$$

Since thermodynamically^{6,124,125} ϕ , η , and ϵ_{ij} are independent of $\dot{\sigma}_{ij}$ and \dot{T} ,

$$\epsilon_{ij} = \partial\phi/\partial\sigma_{ij}, \quad \eta = -\partial\phi/\partial T \quad (A4) \quad (A5)$$

Onsager's reciprocal relation implies sufficient continuity of ϕ that the order of partial differentiation can be interchanged. Thus, the following equality must be satisfied:

* Since the Lagrangian formulation is used, this unit-reference-state volume basis is equivalent to using a unit-mass basis, but it has the advantage of eliminating the symbol for reference-state density in numerous subsequent equations.

$$\left. \frac{\partial}{\partial \sigma_{ij}} \right| \left. \frac{\partial}{\partial T} \left(\frac{\partial \phi}{\partial \sigma_{ij}} \right) \right|_T = \left. \frac{\partial}{\partial T} \right| \left. \frac{\partial}{\partial \sigma_{ij}} \left(\frac{\partial \phi}{\partial \sigma_{ij}} \right) \right|_{\sigma_{ij}}$$

or

$$\left. \frac{\partial}{\partial \sigma_{ij}} \right| \left. \frac{\partial \epsilon_{ij}}{\partial T} \right|_T = \left. \frac{\partial}{\partial T} \right| \left. \frac{\partial \epsilon_{ij}}{\partial \sigma_{ij}} \right|_{\sigma_{ij}} \quad (A6)$$

To obtain constitutive equations which are linear in stress, the free-energy function is assumed to have the following form:

$$\phi = B_1(T)J_1^2 + B_2(T)J_2 + C_1(J_1, T)(J_1)(T - T_0) + F(T) \quad (A7)$$

where T_0 is the temperature at the relaxation state (i.e., the temperature at which the material is free of strain), B_1 and B_2 are temperature-dependent elastic coefficients, C_1 is the usual thermal-expansion coefficient, F is an arbitrary function of temperature only (detailed form selected to represent the nonlinear dependence of specific heat at constant volume on temperature) and J_1 and J_2 are stress invariants defined as follows:

$$J_1 \triangleq \sigma_{ii}, J_2 \triangleq (1/2)\delta_{lm}^{ij}\sigma_{il}\sigma_{jm} \quad (A8)$$

where $i, j, l, m = 1, 2, 3$ and δ_m^{ij} is the generalized Kronecker delta given by:

$$\delta_{lm}^{ij} = \begin{cases} +1 & \text{if } i, j \text{ form an even permutation of } l, m \\ -1 & \text{if } i, j \text{ form an odd permutation of } l, m \\ 0 & \text{if } i, j \text{ do not form a permutation of } l, m \end{cases}$$

The form of the C_1 term in Eq. (A7) implies the existence of a relaxation state, a point which has been questioned by Eckart,²⁵ who offered no specific alternative to use in constructing constitutive relations.

In view of Eq. (A4)

$$\epsilon_{ij} = (\partial\phi/\partial J_1)(\partial J_1/\partial\sigma_{ij}) + (\partial\phi/\partial J_2)(\partial J_2/\partial\sigma_{ij}) \quad (A9)$$

Differentiation of Eq. (A8) yields

$$\partial J_1/\partial\sigma_{ij} = \delta_{ij}, \quad \partial J_2/\partial\sigma_{ij} = \delta_{ij}J_1 - \sigma_{ij} \quad (A10)$$

where δ_{ij} is the simple Kronecker delta (takes values of unity for $i = j$, zero for $i \neq j$).

Inserting Eqs. (A7) and (A10) into Eq. (A9), one obtained

$$\begin{aligned} \epsilon_{ij} = & 2B_1(T)J_1\delta_{ij} + B_2(T)(\delta_{ij}J_1 - \sigma_{ij}) \\ & + \delta_{ij}(T - T_0)\partial(C_1J_1)/\partial J_1 \end{aligned} \quad (A11)$$

or

$$\begin{aligned} \epsilon_{11} = & 2B_1(T)\sigma_{11} + [2B_1(T) + B_2(T)](\sigma_{22} + \sigma_{33}) \\ & + (T - T_0)\partial(C_1J_1)/\partial\sigma_{11} \end{aligned} \quad (A12)$$

(Similar relations for ϵ_{22} and ϵ_{33}).

and

$$\epsilon_{12} = -B_2(T)\sigma_{12} \quad (A13)$$

(similar relations for ϵ_{23} and ϵ_{31}).

Comparing Eqs. (A12) and (A13) with those of classical elasticity theory, we find

$2B_1 \rightarrow E^{-1}$, where E is Young's modulus

$2B_1 + B_2 \rightarrow -\nu/E$, where ν is Poisson's ratio

$\partial(C_1 J_1)/\partial J_1 \rightarrow \alpha$, lineal coefficient of thermal expansion

To check whether the Onsager requirement, represented by Eq. (A6) is satisfied, the mixed partial derivatives are taken as follows:

$$\begin{aligned} \frac{\partial}{\partial \sigma_{ij}} \left(\frac{\partial \epsilon_{ij}}{\partial T} \right) &= 2 \frac{d B_1}{d T} \delta_{ij} + \frac{d B_2}{d T} (\delta_{ij} - 1) + \delta_{ij} \frac{\partial^2}{\partial J_1 \partial T} [(T - T_0) \partial(C_1 J_1)/\partial J_1] \\ &= \frac{\partial}{\partial T} \left(\frac{\partial \epsilon_{ij}}{\partial \sigma_{ij}} \right) \end{aligned} \quad (A14)$$

Equation (A14) shows that Eq. (A6) is satisfied without placing any restrictions whatsoever on the form of the constitutive functions

$B_1(T)$, $B_2(T)$, $C_1(J_1, T)$, and $F(T)$.

The specific entropy is computed from Eqs. (A5) and (A7) with the following result:

$$\eta = -J_1^2 \frac{d B_1}{d T} - J_2 \frac{d B_2}{d T} - J_1 \partial[(T - T_0) C_1]/\partial T - d F/d T \quad (A15)$$

Since there can be no entropy production during continuous deformation of a perfectly elastic material, the specific entropy must be independent of the stresses. Thus, from Eq. (A15):

$$d B_2/d T = 0 \quad (A16)$$

$$J_1 \frac{d B_2}{d T} + \partial[(T - T_0) C_1]/\partial T = 0 \quad (A17)$$

It can be shown that B_2 is the reciprocal of the shear modulus $G = E/2(1 + \nu)$; thus, Eq. (A16) implies that the shear modulus should be independent of temperature. However, it is an experimentally observed

fact that the shear modulus is temperature dependent. This can be accommodated quite easily by adding a term of the following form to the free-energy function ϕ in Eq. (A7).

$$C_2(J_2, T)(J_2)(T - T_0)$$

In the stress-strain equation, Eq. (A11), this adds a term of the form

$$(\delta_{ij}J - \sigma_{ij})(T - T_0)\partial(C_2J_2)/\partial J_2$$

which is analogous to the deviatoric-thermal-expansion effect considered theoretically and experimentally by Dillon.¹⁷ Addition of this term does not prevent satisfaction of Eq. (A6).

To obtain some useful information from Eq. (A17), use is made of the following relation observed in experiments by Rosenfield and Averbach:¹⁶

$$C_1(\sigma_{kk}, T) = C_{10}(T) + C'_{11}(T)\sigma_{kk}$$

Rosenfield and Averbach used only uniaxial loading and measured C'_{11} only in the direction of that loading. However, it seems intuitively apparent that a stress in direction 1 could affect the thermal expansion in direction 1 only, i.e., since the loading is directional, its effect on C_1 should also be directional. This probably could be proved by functional analysis. However, the present theory is an isotropic one; thus, the preceding equation must be rewritten as its isotropic equivalent:

$$C_1(J_1, t) = C_{10}(t) + C_{11}(t)J_1 \quad (A18)$$

Then Equation (A17) leads to

$$\begin{aligned} J_1 \, dB_1/dT \, Td[(T - T_0)C_{10}]/dT \\ + J_1 \, d[(T - T_0)C_{11}]/dT = 0 \end{aligned} \quad (A19)$$

Again invoking independence of stress, Eq. (A19) implies:

$$d[(T - T_o)C_{10}]/dT = 0 \quad (A20)$$

and

$$dB_1/dT + d[(T - T_o)C_{11}]/dT = 0 \quad (A21)$$

Integration of Eq. (A20) yields:

$$(T - T_o)C_{10}(T) = \text{Const.} \quad (A22)$$

Equation (A22) does not appear to be realistic; this suggests that further work on this topic is required.

Equation (A21) expresses an interrelationship between B_1 and C_{11} . Since the experiments of Rosenfield and Averbach were conducted at room temperature only, the validity of Eq. (A21) cannot be checked with experimental data at present. Table 1 lists some sets of specific forms for C_{11} and B_1 which satisfy Eq. (A21).

Since $B_1 = (2E)^{-1}$, Eq. (2) in the body of the report can be put in the following form:

$$C_{11} = 2 dB_1/dT \quad (A23)$$

Thus, Eq. (A23) corresponds to a g value of 2, where g is defined as follows:

$$g \triangleq C_{11}/(dB_1/dT) \quad (A24)$$

It is noted that the form of Eq. (A23) is identical to Cases 2-4 in Table 1, even though the coefficient g differs considerably. It is

TABLE 1
SOME SETS OF SPECIFIC FORMS OF COEFFICIENTS B_1 AND C_{11} WHICH SATISFY
EQUATION (A21)

Set No.	B_1^*	C_{11}^*	$g(T) \triangleq C_{11}/(dB_1/dT)$
1	K_1	$K_2/(T - T_0)$	∞
2	$K_4 - K_3T$	K_3	-1
3	---	$K_5 e^{-k/T}$	$-[1 + (T - T_0)k/T^2]^{-1}$
4	---	$K_6 T^p$	$-[1 + (T - T_0)p/T]^{-1}$

* K_i , k , p are constants

noted that for temperatures near to the strain-free temperature (t_0), Cases 2-4 predict $g \approx -1$. However, Rosenfield and Averbach's experiments for five metals gave a value of g within 3% of 2 (although individual variations for specific metals differed from 2 by 6% to 100%).

Apparently Rosenfield and Averbach made a mathematical error in applying Eq. (A6), and in doing so, they obtained the interrelationship Eq. (2). This is contrary to current thinking in thermodynamics that Onsager's relation should not place numerical restrictions on the constitutive equation coefficients, but rather should be used only in determining the general form of the constitutive equations. Nevertheless, it is puzzling that Eq. (A23) agrees with experimental results better than with the values of Cases 2-4 in Table 1.

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<p>The historical development of the foundations of thermomechanics is reviewed, with emphasis placed upon the critical contribution of each investigator. The theories are discussed in terms of their relevance to real materials in the important high-velocity regime which lies between the low and intermediate velocity regime (which involves essentially isothermal elastic and plastic wave propagation) on one hand and the ultrahigh-velocity regime (in which a hydrodynamic description of the material behavior is adequate) on the other. Various facets of high-velocity wave propagation in various materials involve elastic, plastic, viscous, and thermal effects on a macroscopic scale and perhaps on a microscopic scale. Evaluations are made from the standpoint of thermodynamics as well as classical mechanics.</p> <p>Using fundamental principles of thermodynamics and mechanics, thermomechanically coupled linear energy and constitutive equations are derived for the elastic solid with micro unit cells discussed by Mindlin.</p> <p>Equations of motion for the microstructure are found for the large amplitude case where Eulerian and Lagrangian formulations are not identical.</p>		

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